

METHOD FOR RESIDUAL FORM IN MOLECULAR MODELING

ABSTRACT OF THE DISCLOSURE

The Residual Form of the equations of motion of a molecular model is used to reduce the computational load by a factor of approximately 7 as compared to the conventional Direct Form (not including the force computations). Implicit integrators are used with the Residual Form, especially L-stable integrators, such as implicit Euler and Radau5. A preferable molecular model is an Order (N), torsion angle, rigid multibody system.

PA 3180742 v1